Supplementary Material

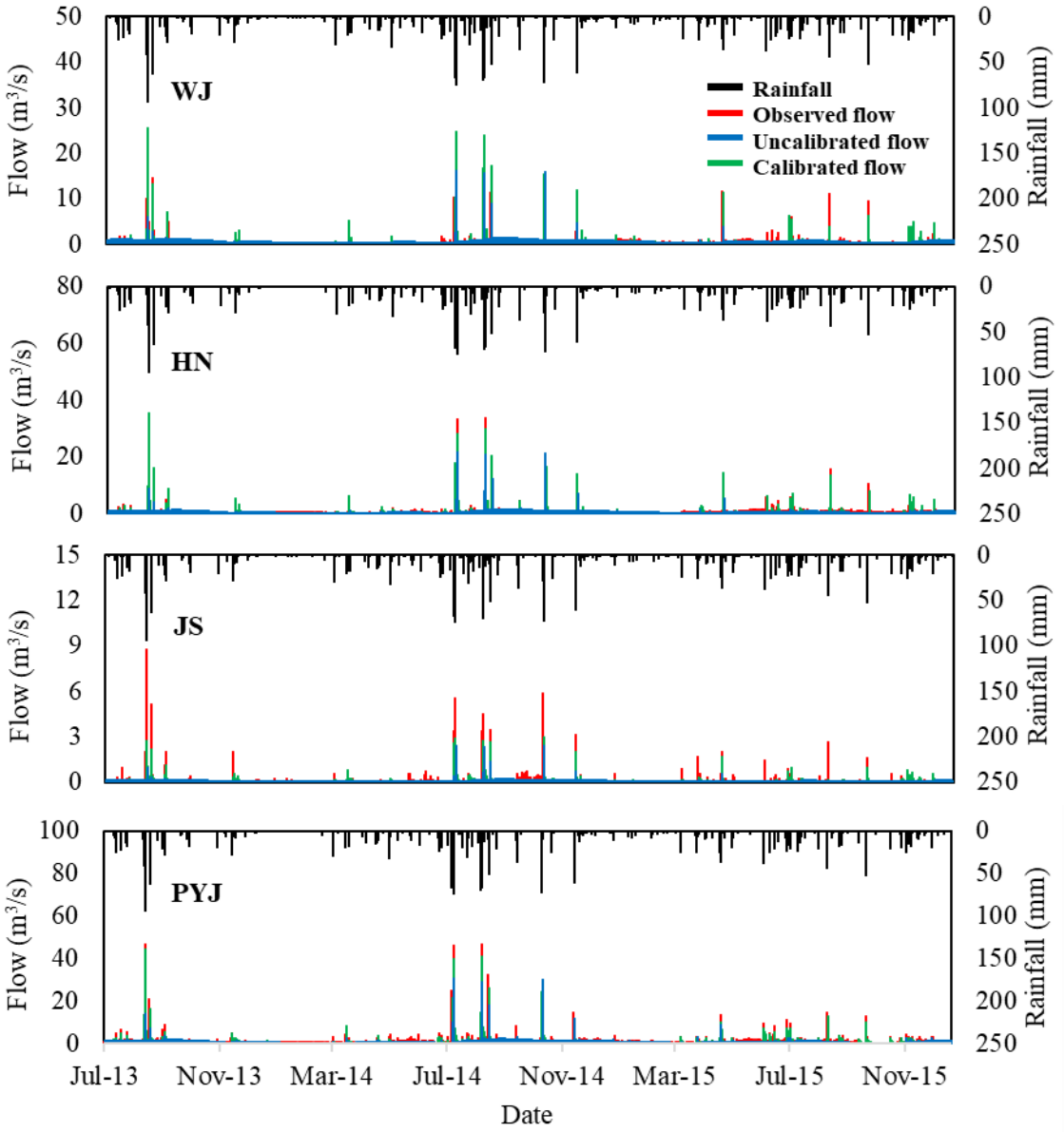


Figure S1. Comparison of daily streamflow predicted using the mechanistic models (i.e., uncalibrated and calibrated SWAT models) and observed during the training period (July 12, 2013, to December 31, 2015).

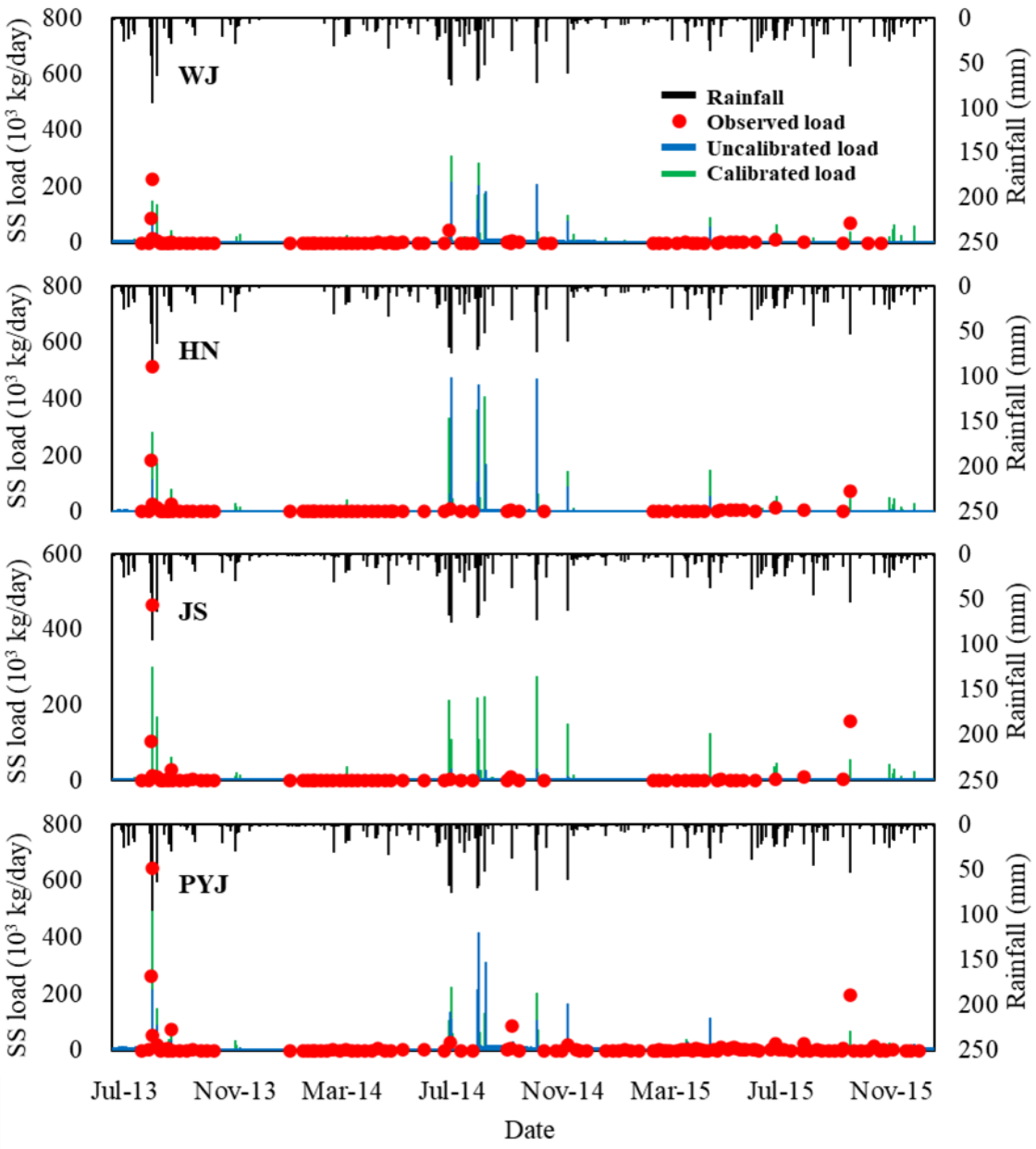


Figure S2. Comparison of daily SS loads predicted using the mechanistic models (i.e., uncalibrated and calibrated SWAT models) and observed during the training period (July 12, 2013, to December 31, 2015).

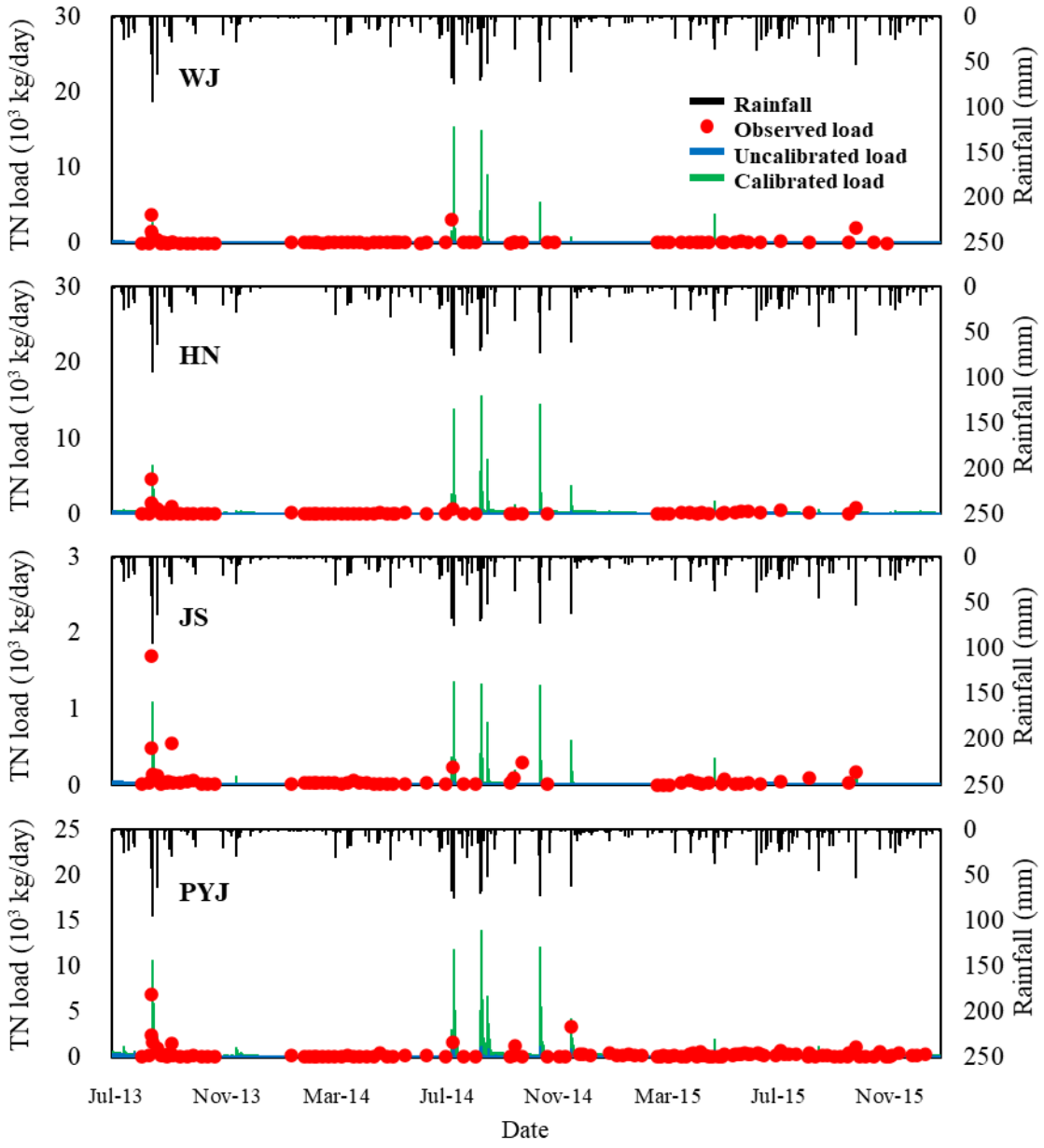


Figure S3. Comparison of daily TN loads predicted using the mechanistic models (i.e., uncalibrated and calibrated SWAT models) and observed during the training period (July 12, 2013, to December 31, 2015).

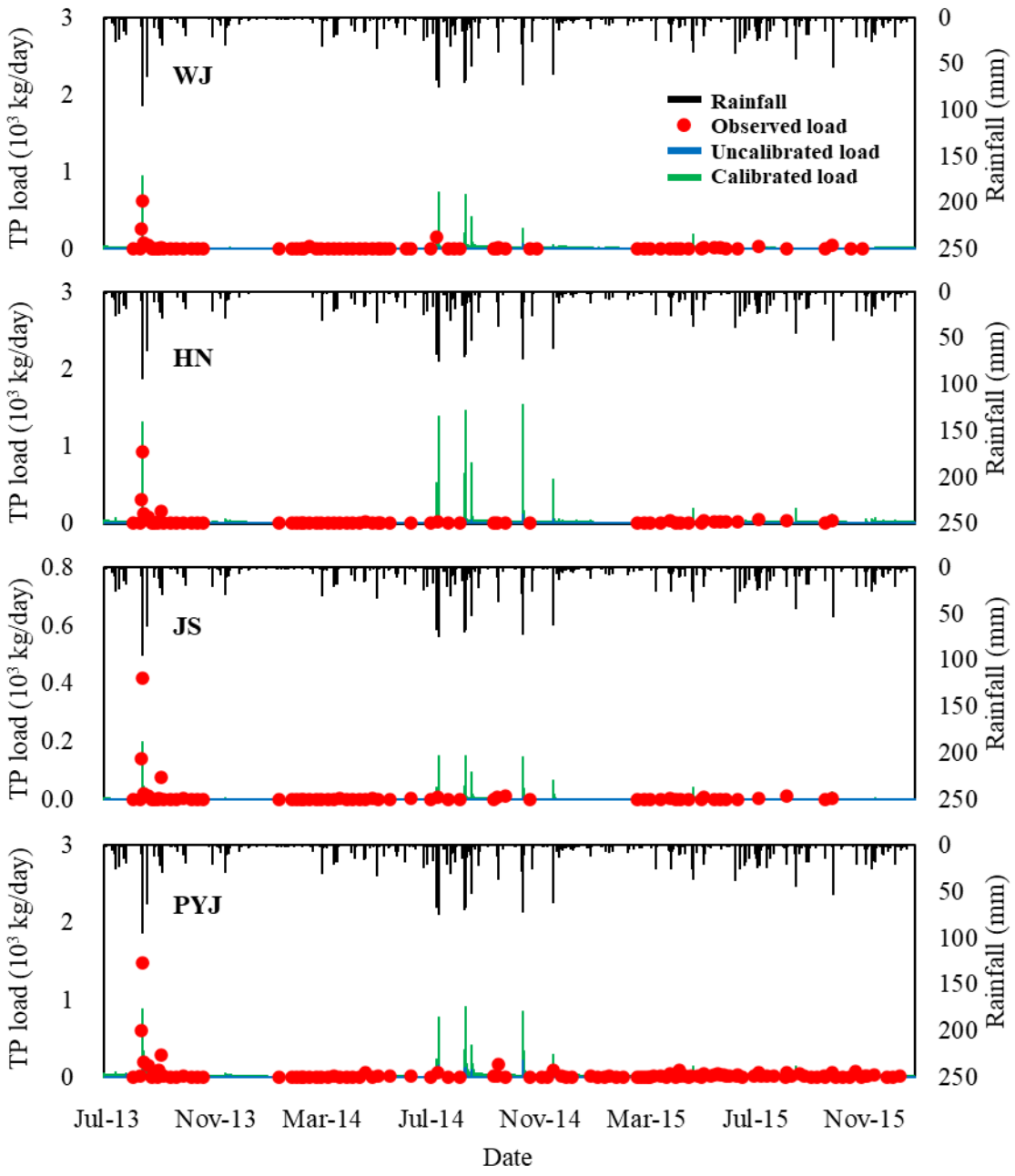
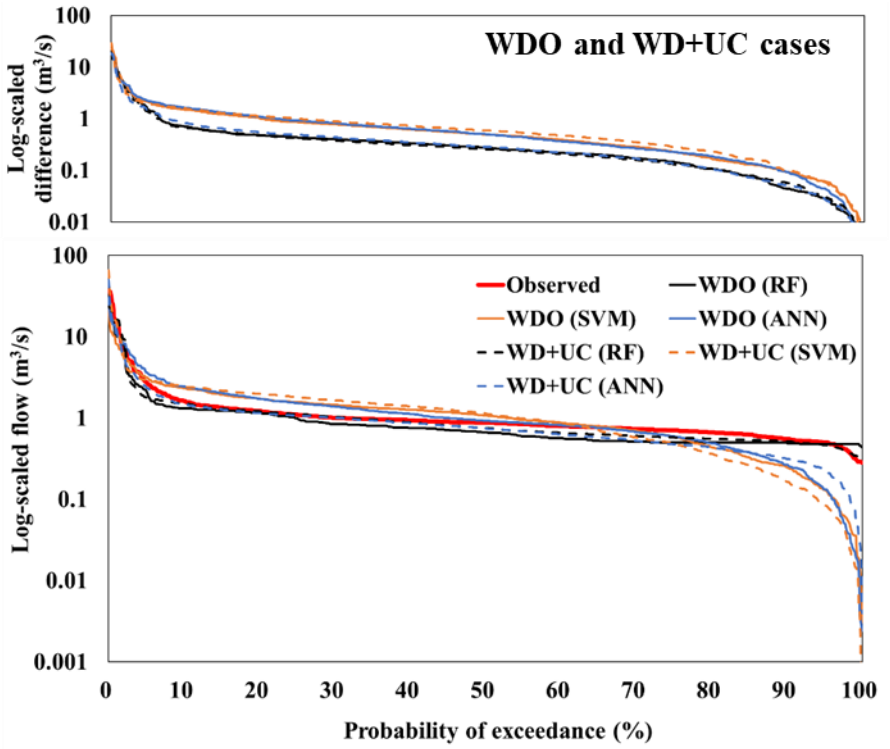
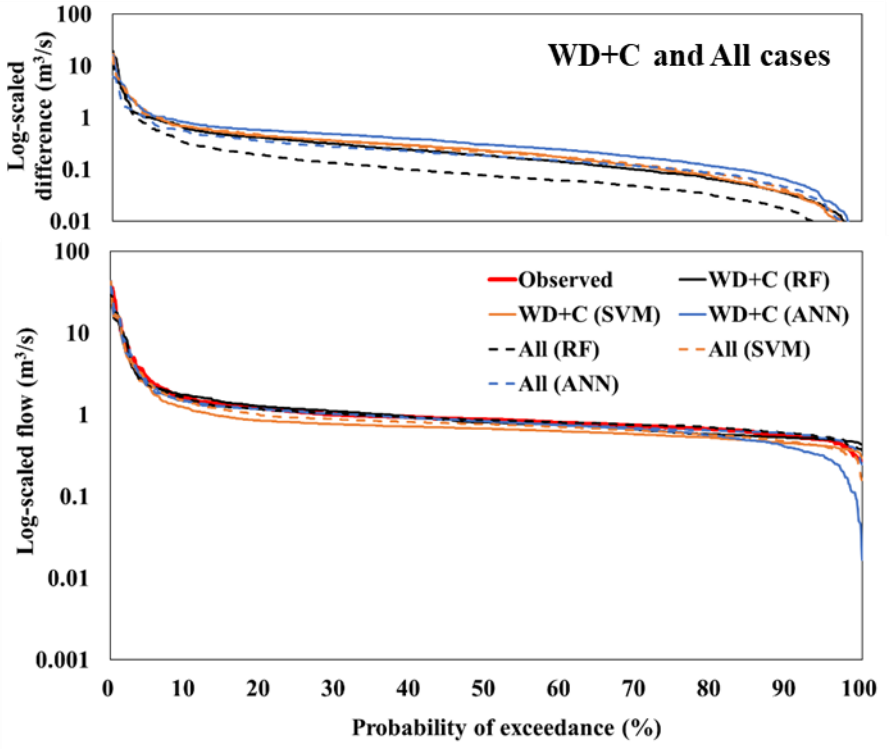
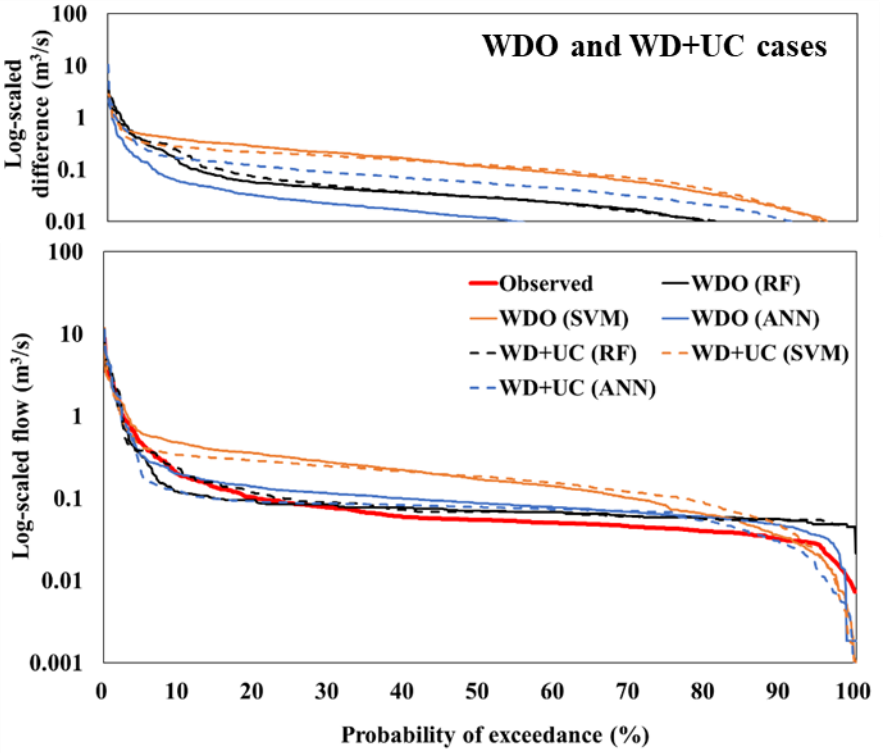


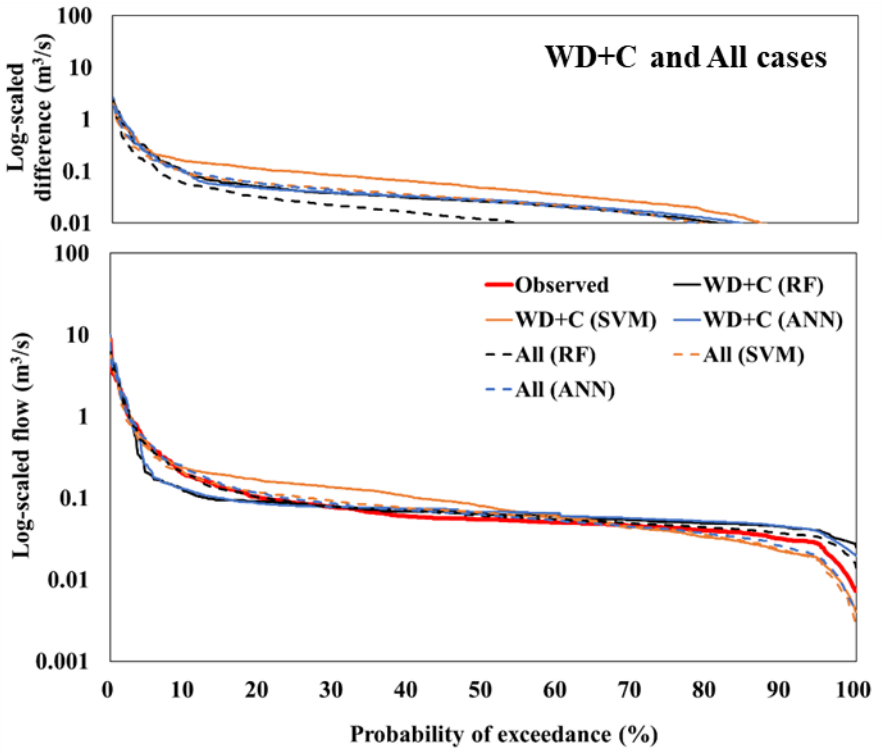
Figure S4. Comparison of daily TP loads predicted using the mechanistic models (i.e., uncalibrated and calibrated SWAT models) and observed during the training period (July 12, 2013, to December 31, 2015).



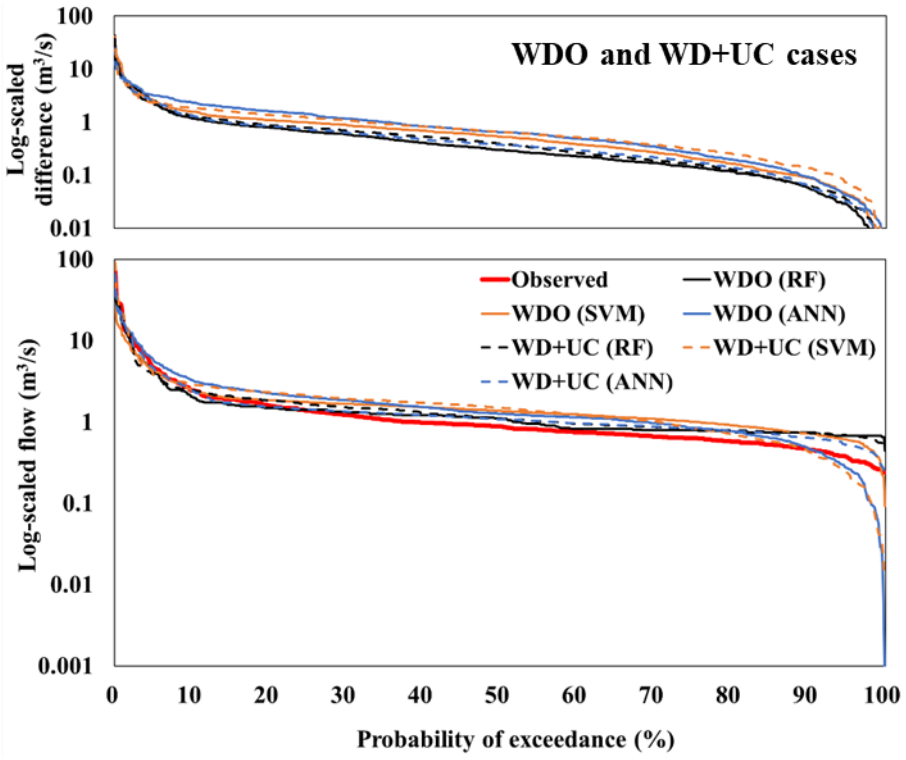


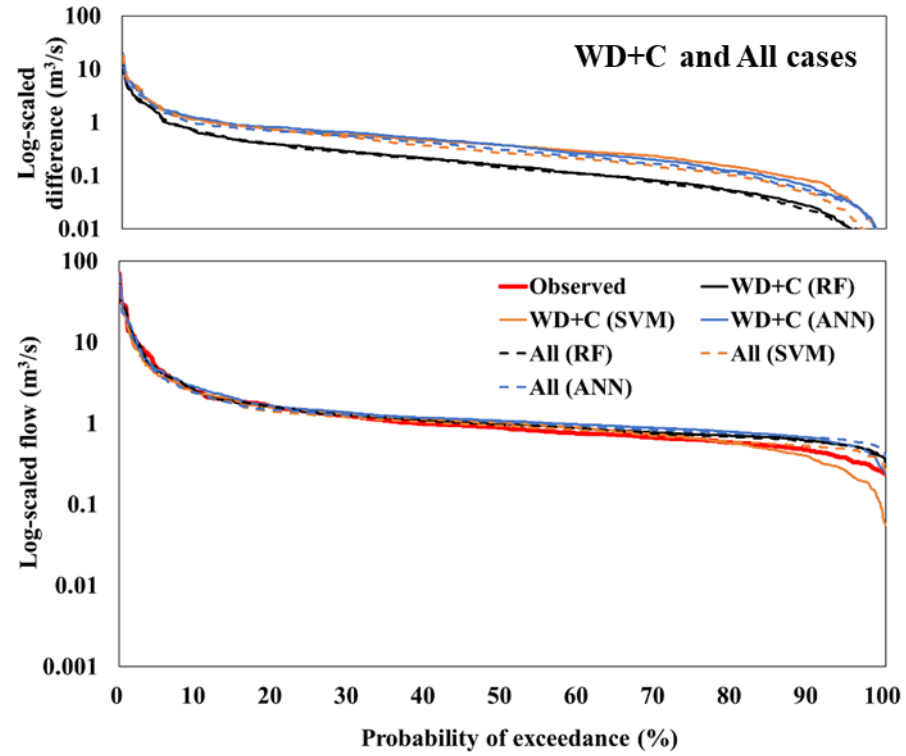
(a) Log-scaled flow duration curves at the outlet of the HN watershed



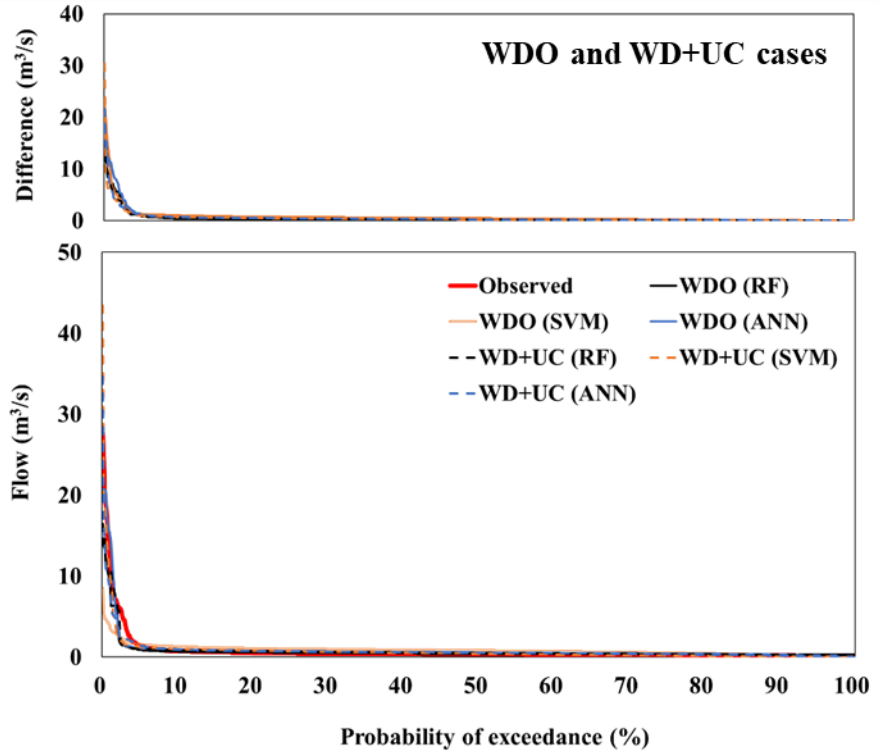


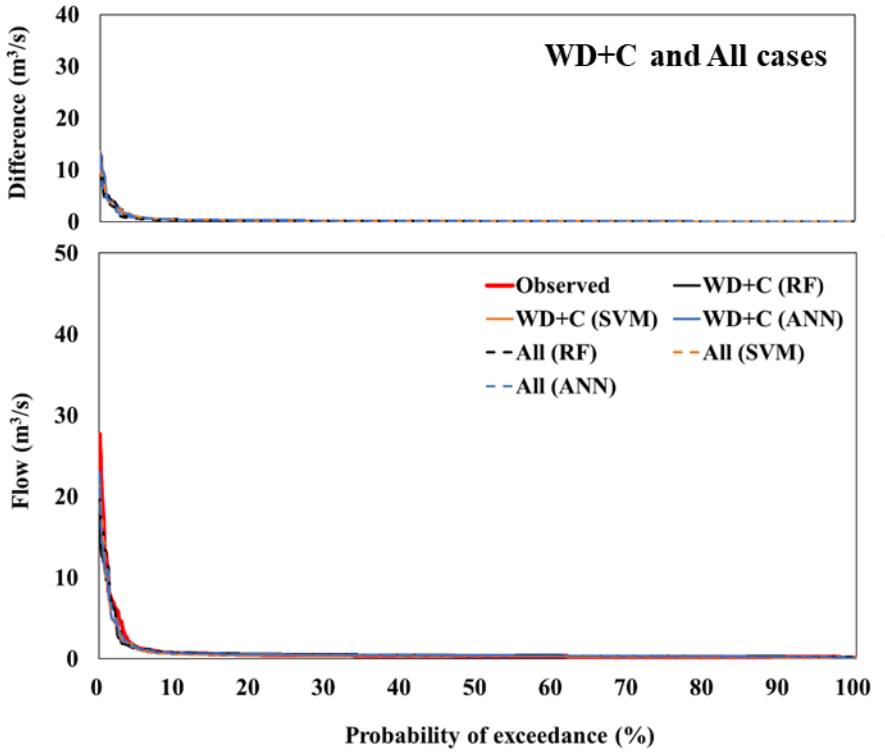
(b) Log-scaled flow duration curves at the outlet of the JS watershed



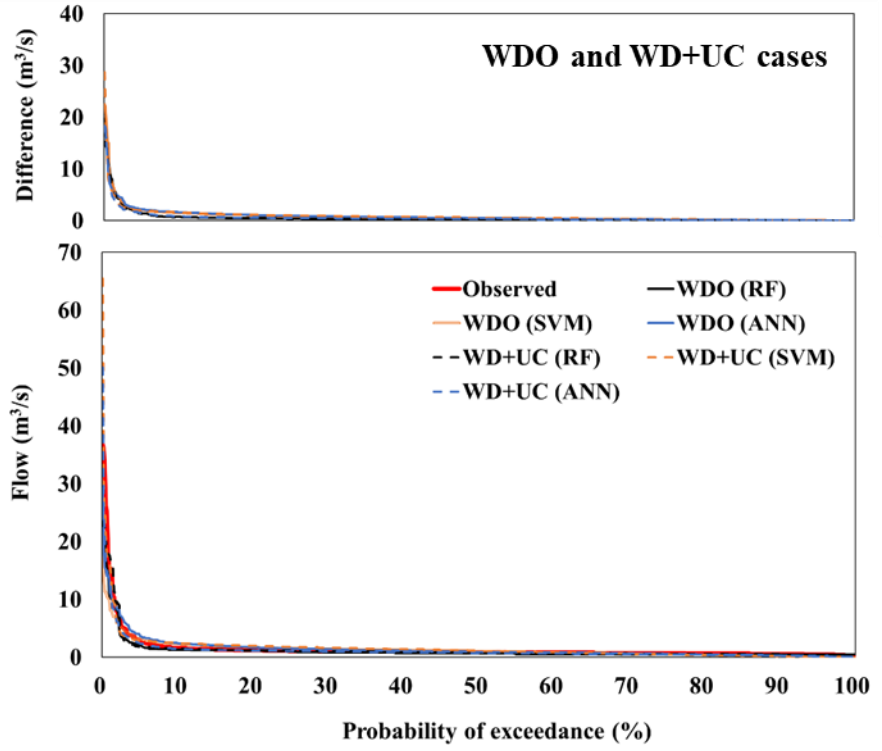


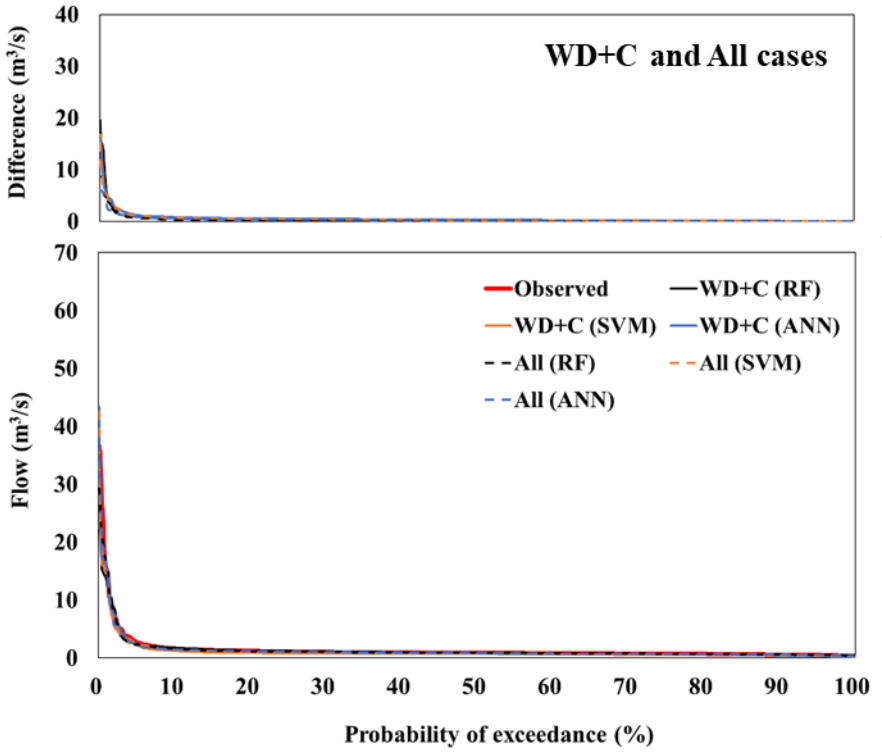
(c) Log-scaled flow duration curves at the outlet of the PYJ watershed



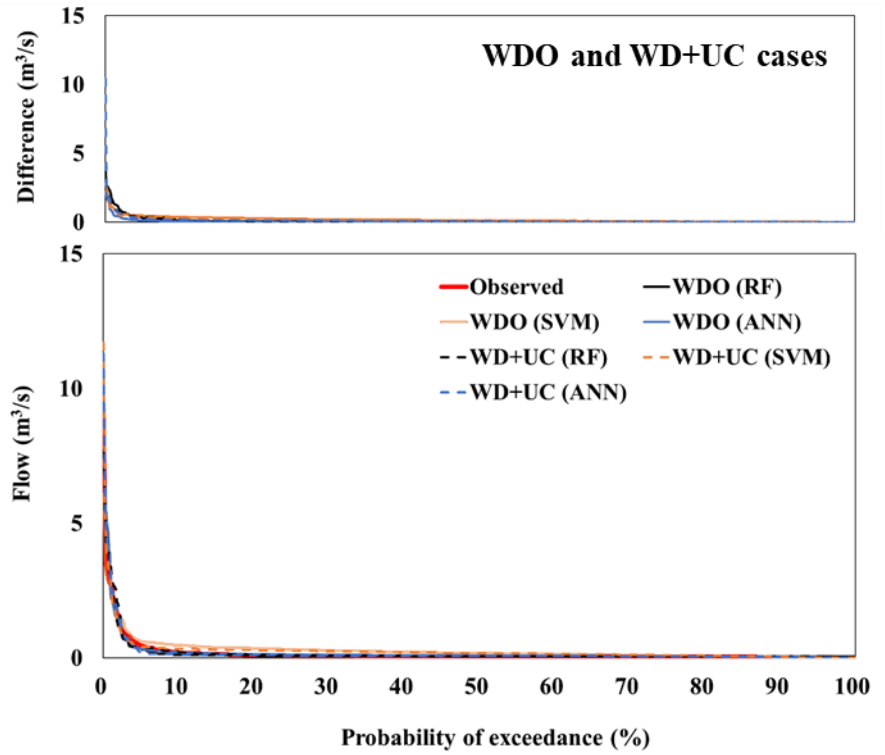


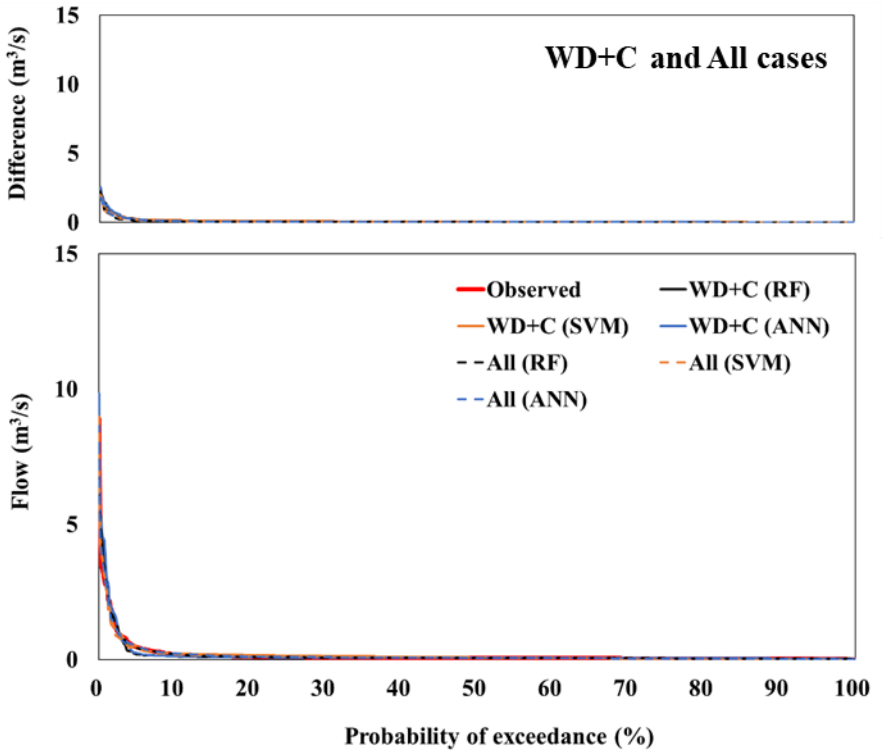
(d) Normal-scaled flow duration curves at the outlet of WJ watershed



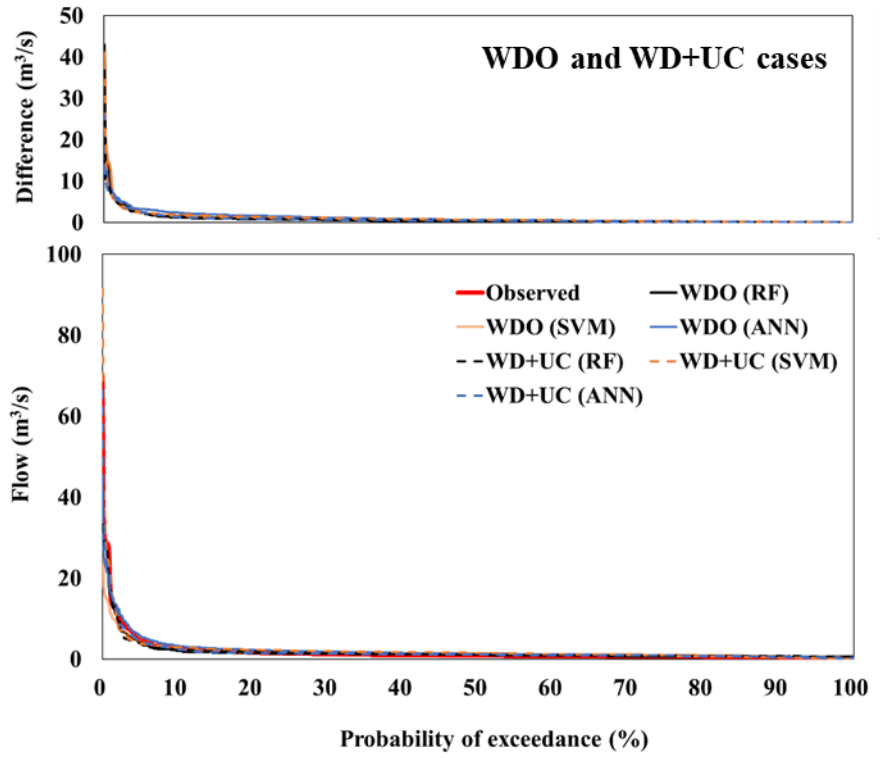


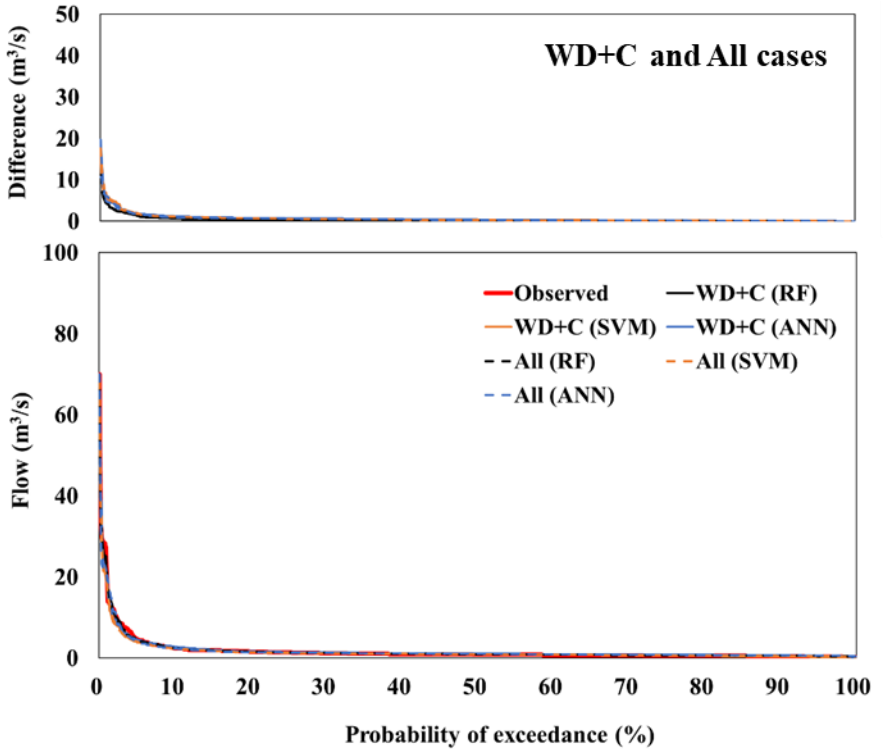
(e) Normal-scaled flow duration curves at the outlet of HN watershed





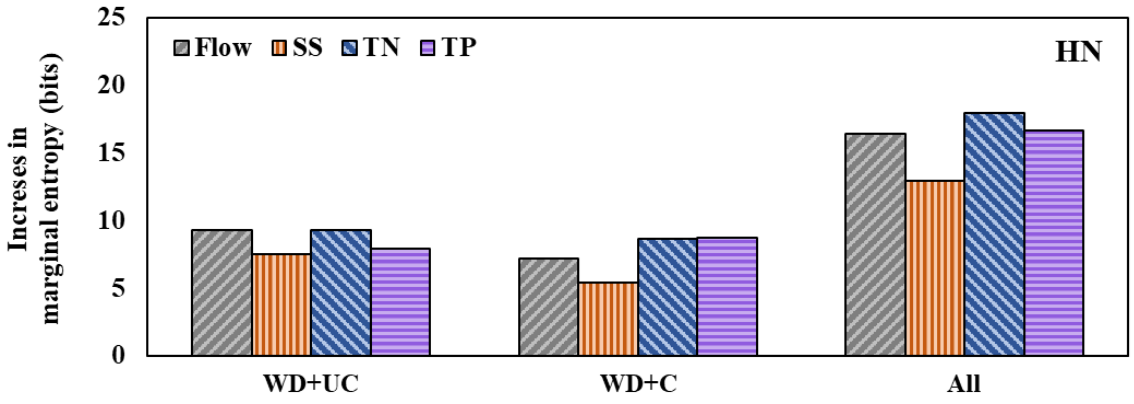
(f) Normal-scaled flow duration curves at the outlet of JS watershed



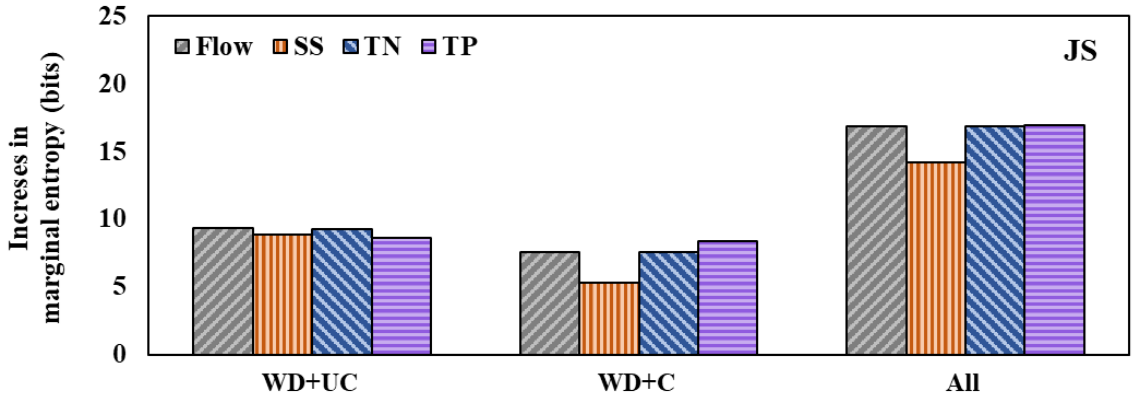


(g) Normal-scaled flow duration curves at the outlet of PYJ watershed

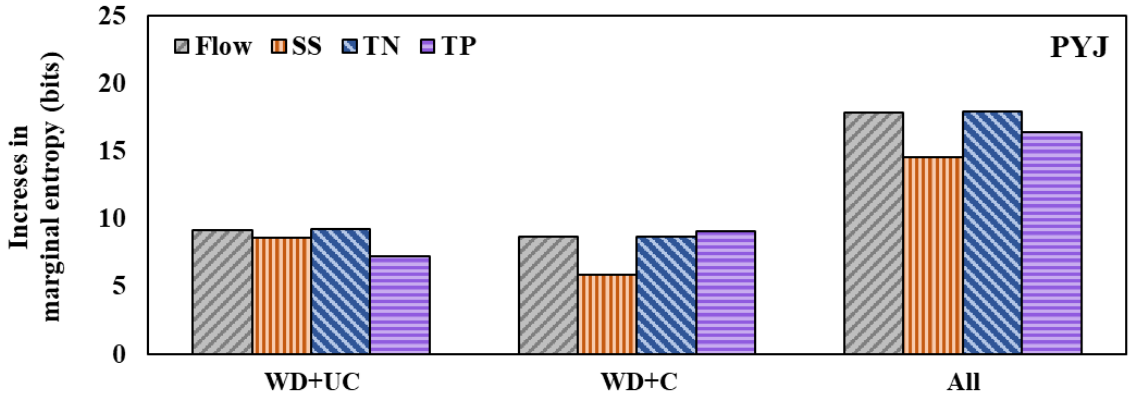
Figure S5. Comparison between observed and ML-predicted flow duration curves (FDC). (a, b, and c) represent the FDC in log scale at the outlets of the HN, JS, and PYJ watersheds. The FDC at the WJ watershed is presented in Figure 5 in the manuscript. (d, e, f, and g) represent the FDC in normal scale at the outlets of WJ, HN ,JS, and PYJ watersheds.



(a) HN watershed

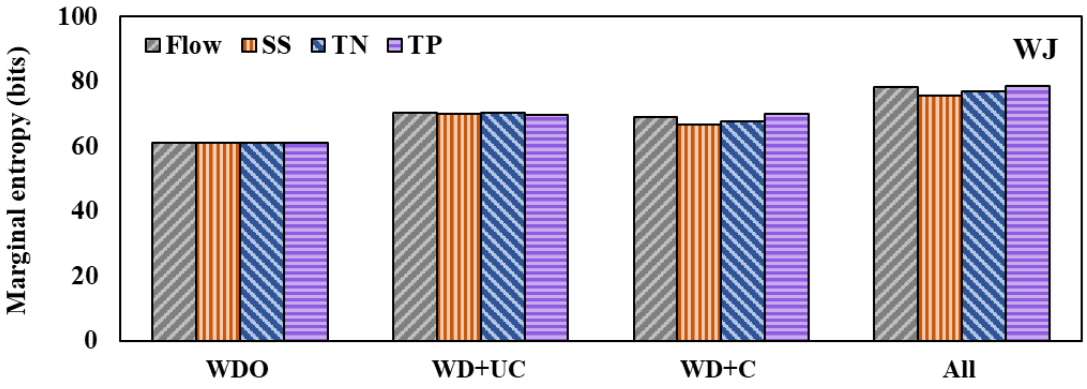


(b) JS watershed

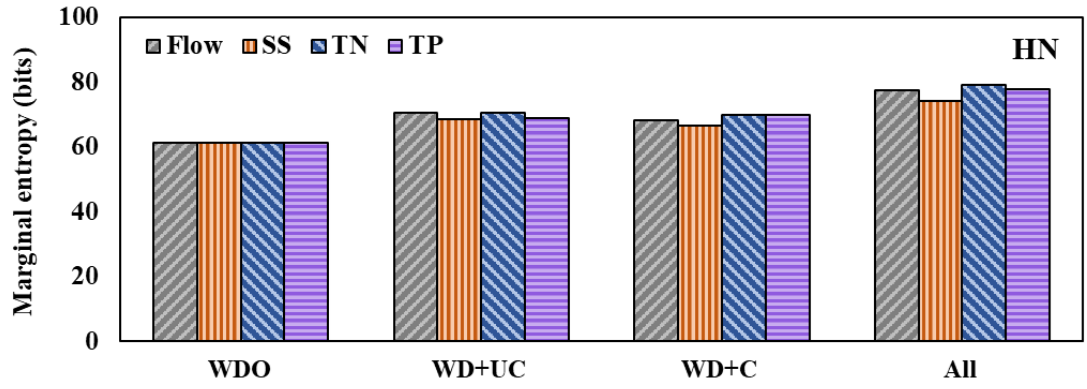


(C) PYJ watershed

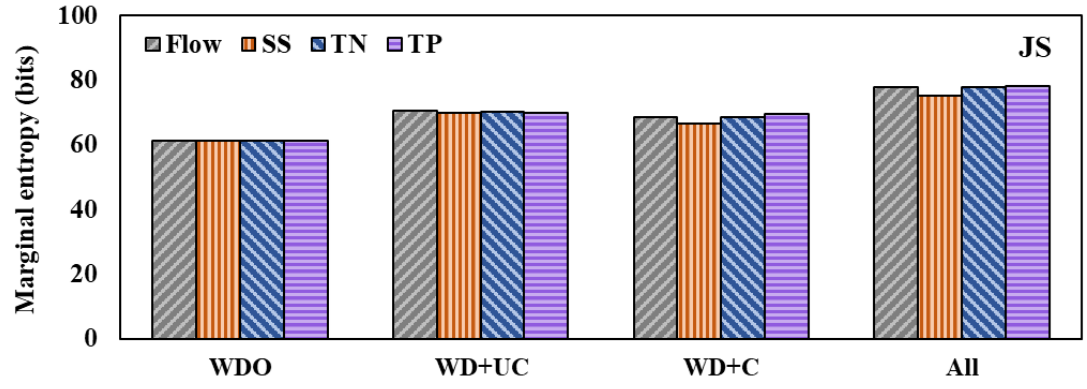
Figure S6. Increases in marginal entropy due to the addition of training data sets from different watersheds (HN, JS, and PYJ). The WDO training data set serves as the baseline for this comparison.



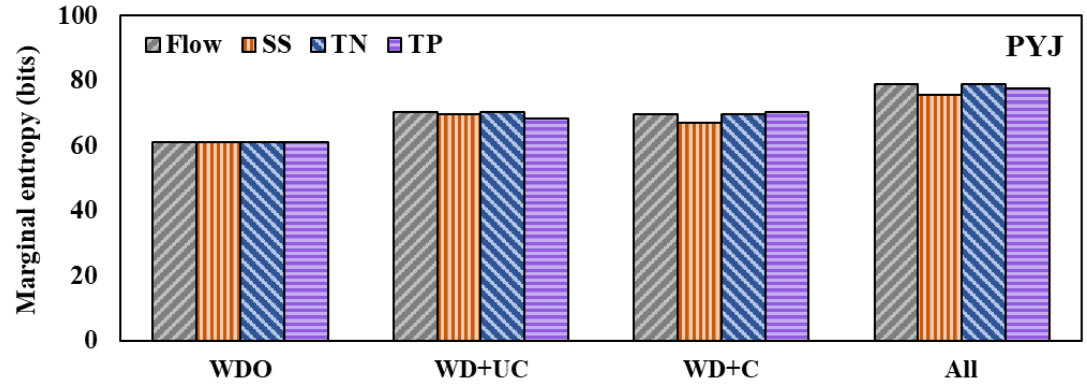
(a) WJ watershed



(b) HN watershed

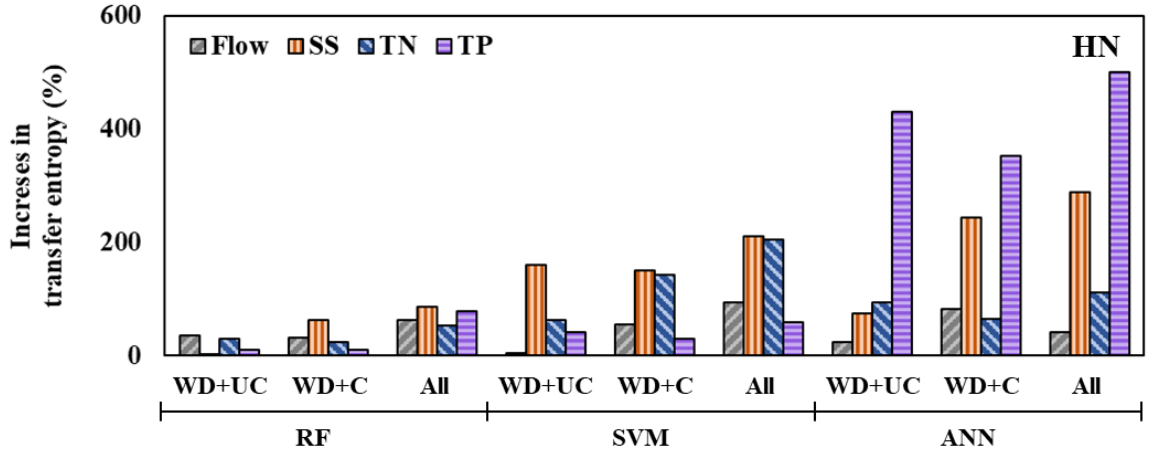


(c) JS watershed

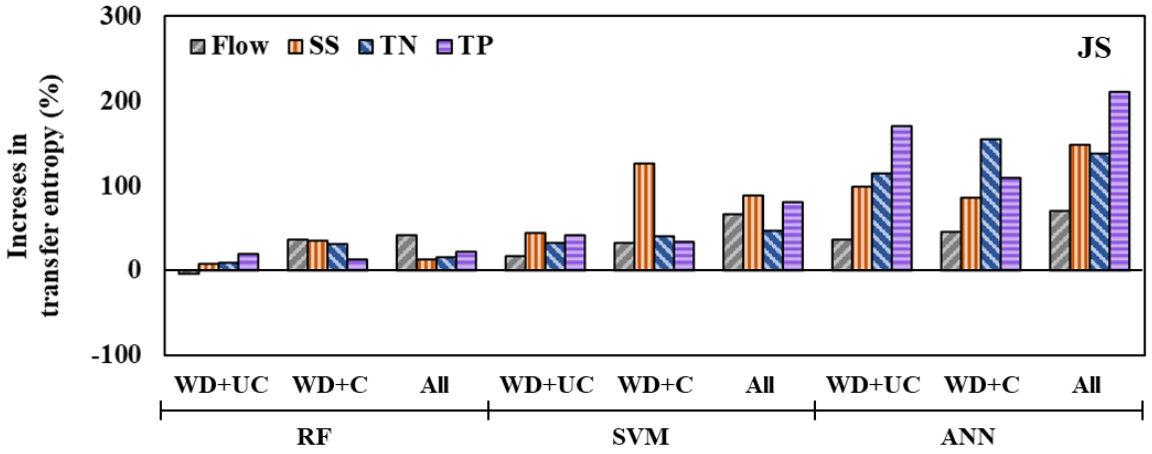


(d) PYJ watershed

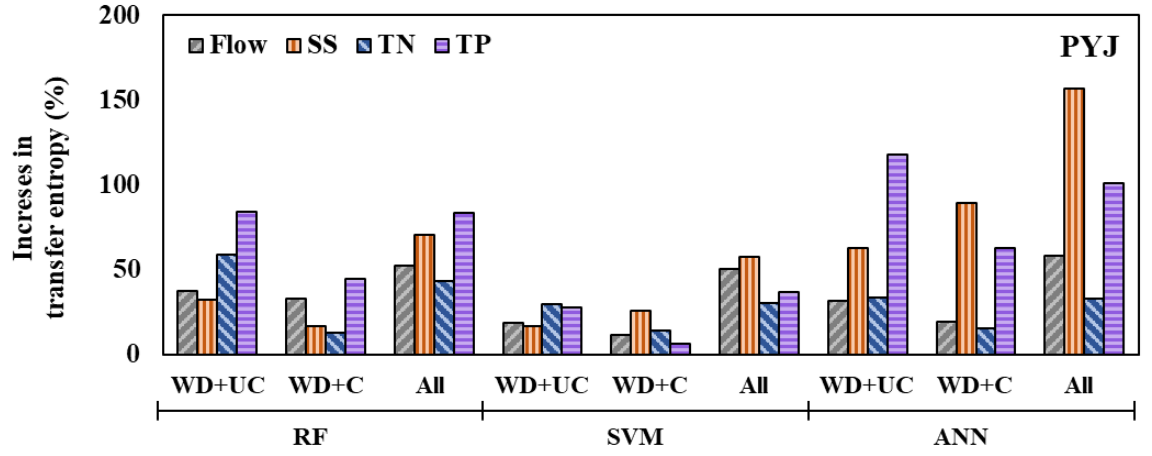
Figure S7. Marginal entropy of the training data sets by the watersheds with different target variables.



(a) HN watershed

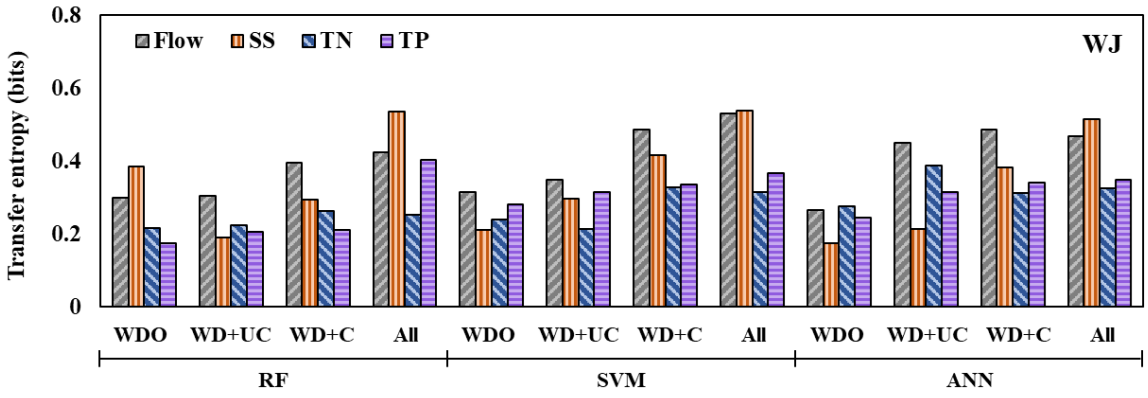


(b) JS watershed

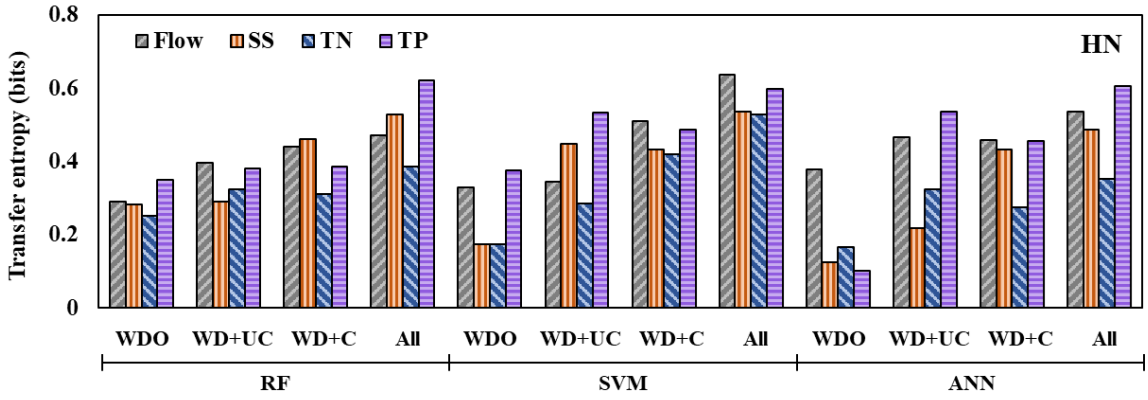


(C) PYJ watershed

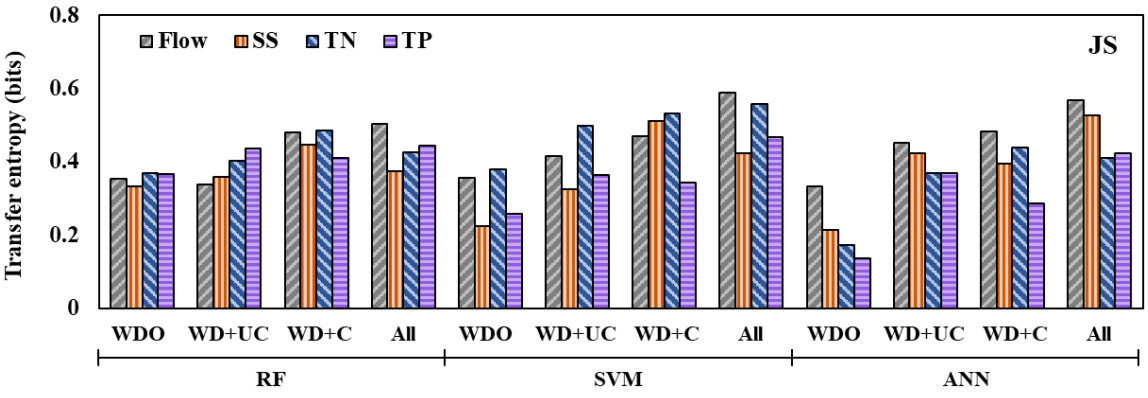
Figure S8. Increases in transfer entropy due to the addition of training data sets from different watersheds (HN, JS, and PYJ). The WDO training data set serves as the baseline for this comparison.



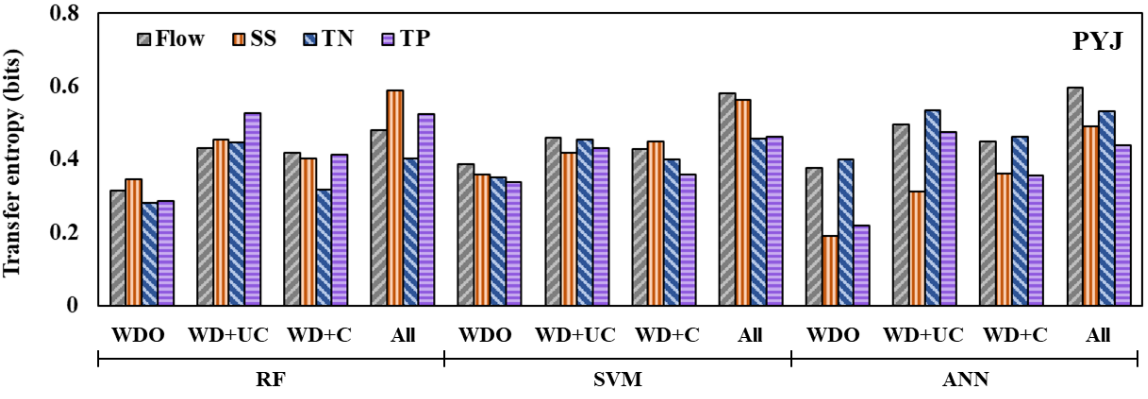
(a) WJ watershed



(b) HN watershed

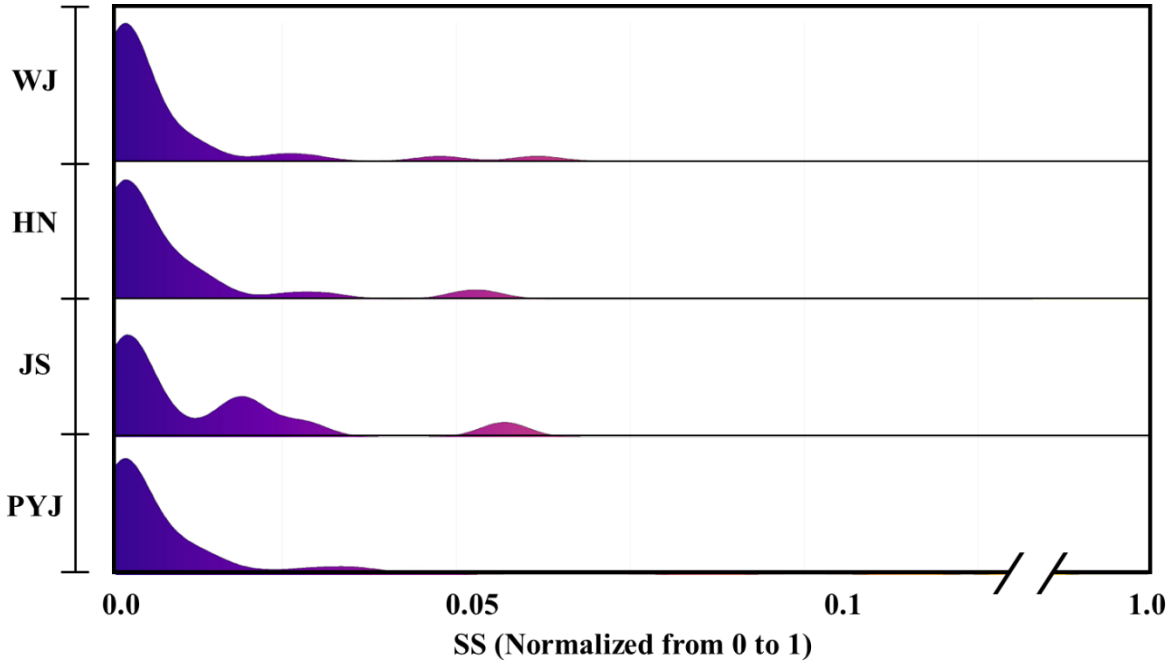


(c) JS watershed

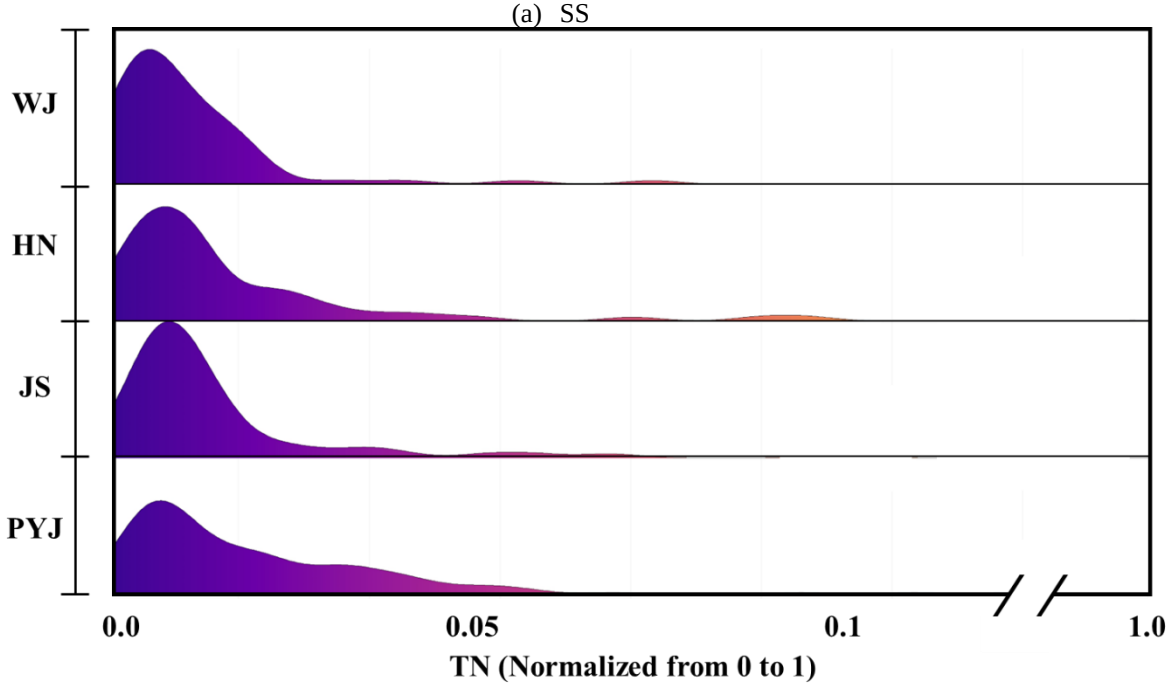


(d) PYJ watershed

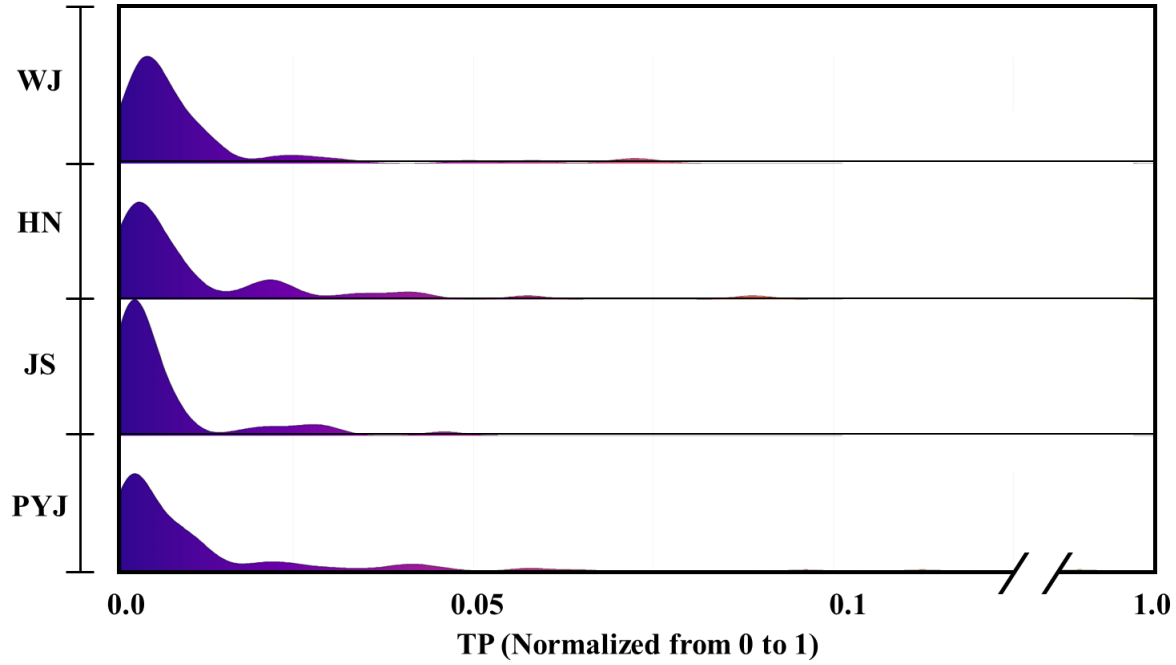
Figure S9. Transfer entropy of the training data sets by the machine learning algorithms with different target variables.


WJ
HN
JS
PYJ
0.0
0.05
0.1
1.0
SS (Normalized from 0 to 1)

(a) SS


WJ
HN
JS
PYJ
0.0
0.05
0.1
1.0
TN (Normalized from 0 to 1)

(b) TN



(C) TP

Figure S10. Density (or frequency) distributions of observed SS, TN, and TP concentrations during the training period. The concentrations were normalized from 0 to 1 for each watershed.

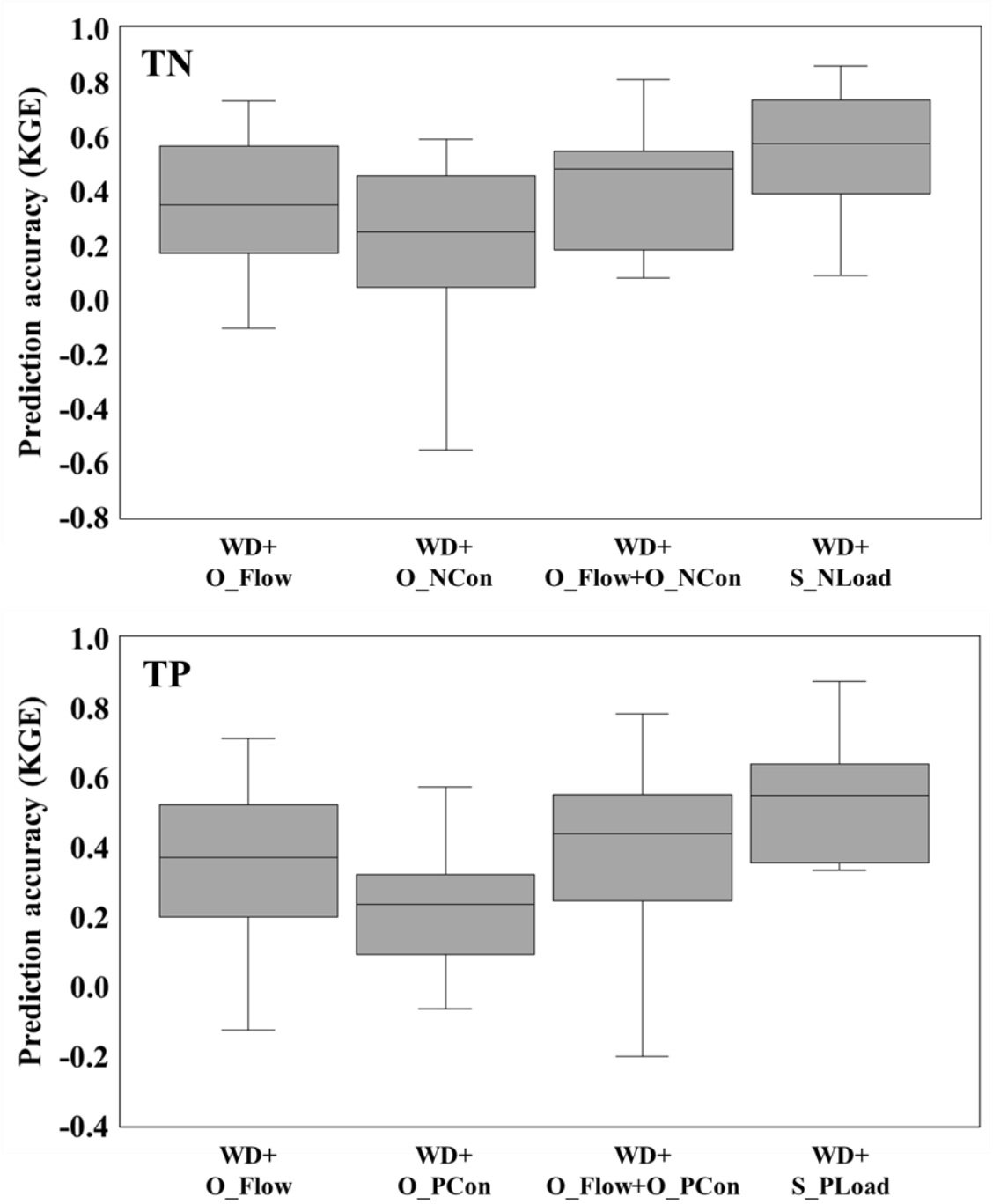


Figure S11. Comparison of TN and TP prediction accuracy (KGE) for ML models trained with different input data combinations across the four study watersheds. Each box and whisker plot represents the variation in prediction accuracy by watershed (WJ, HN, JS, and PYJ) and ML algorithm (RF, SVM, and ANN).

Table S1. Land use and cover statistics of the study watersheds.

Study Watersheds	Average Slope (%)	Land uses and Covers (km^2)					
		Urban	**Field**	**Paddy field**	**Forest**	**Other**	**Total**
WJ	6.43	1.88 (5%)	6.63 (19%)	14.77 (43%)	8.45 (24%)	3.02 (9%)	34.75 (100%)
HN	5.49	5.68 (13%)	9.28 (21%)	17.19 (38%)	9.33 (21%)	3.62 (8%)	45.09 (100%)
JS	4.39	2.40 (31%)	1.21 (15%)	2.07 (26%)	1.73 (22%)	0.42 (5%)	7.83 (100%)
PYJ	4.85	11.46 (19%)	22.36 (36%)	11.23 (18%)	11.45 (19%)	4.90 (8%)	61.40 (100%)

Table S2. Management practice application schedules and rates considered in the SWAT modelling.

Month	Day	Operation	Value	Crop
5	1	Fertilizer application	67.5 kg ha-1 (N) 45.0 kg ha-1 (P)	Rice
6	1	Plant/begin growing season		
7	10	Fertilizer application	22.5 kg ha-1 (N)	
10	1	Harvest and kill operation		

Table S3. Types of calibration parameters and their values in the SWAT modeling.

Variables	Parameters	Calibrated Values			
		WJ	HN	JS	PYJ
Flow	CN2.mgt	58.0	51.4	81.5	55.0
	ALPHA_BF.gw	0.02	0.58	0.12	0.23
	GW_DELAY.gw	424.6	470.4	414.6	34.2
	GW_REVAP.gw	0.12	0.15	0.09	0.12
	GWQMN.gw	3121	1671	404.2	125.0
	EPCO.bsn	0.20	0.55	0.33	0.19
	ESCO.bsn	0.57	0.98	0.01	0.39
	SUR_LAG.bsn	3.66	7.22	1.47	19.8
	OV_N.hru	0.23	0.23	0.28	0.14
	CH_N2.rte	0.15	0.18	0.17	0.27
	CH_K2.rte	85.3	5.42	21.3	0.83
	SOL_AWC.sol	0.04	0.09	0.03	0.51
SS	USLE_P.mgt	0.33	0.22	0.29	0.81
	SPCON.bsn	0.005	0.0004	0.008	0.003
	SPEXP.bsn	1.42	1.24	1.08	1.43
	ADJ_PKR.bsn	1.46	1.15	0.97	0.70
	EROS_SPL.bsn	1.08	3.00	1.40	2.14
	EROS_EXPO.bsn	2.43	1.94	1.78	2.08
	C_FACTOR.bsn	0.07	0.30	0.28	0.01
	RILL_MULT.bsn	0.57	0.98	0.54	1.97
	PRF.bsn	1.47	0.40	0.17	1.71
	CH_D50.bsn	84.5	60.3	45.0	54.1
	USLE_K.sol	0.64	0.65	0.47	0.65
	CH_COV1.rte	0.53	0.23	0.68	0.71
	CH_COV2.rte	0.64	0.31	0.65	0.36
	USLE_C.dat	0.49	0.40	0.34	0.42
TN	BIOMIX.mgt	0.13	0.68	0.15	0.67
	LAT_ORGN.gw	104.9	191.9	58.7	26.2
	RCN.bsn	3.68	4.85	11.0	9.68
	N_UPDIS.bsn	12.4	17.0	74.8	85.3
	NPERCO.bsn	0.59	0.17	0.86	0.29
	CMN.bsn	0.003	0.003	0.002	0.002
	CDN.bsn	2.05	0.60	2.66	0.60
	SDNCO.bsn	0.35	0.94	0.76	0.16
	ERORGN.hru	0.41	4.91	0.13	0.25
	RS4.swq	0.04	0.01	0.09	0.05
	BC3.swq	0.35	0.25	0.22	0.35
TP	LAT_ORGP.gw	33.1	8.50	2.10	1.00
	P_UPDIS.bsn	30.1	30.0	6.55	0.90
	PPERCO.bsn	15.1	17.1	16.3	12.5
	PSP.bsn	0.56	0.61	0.36	0.69
	ERORGP.hru	0.03	0.89	0.05	0.48
	RS5.swq	0.04	0.04	0.09	0.03
	BC4.swq	0.46	0.49	0.30	0.11

Table S4. Descriptive statistics of observations and training data.

Variables	WS*	Unit	Min	Mean	Max	Std. Dev. **	CoV (%)***	Number of observations
P	-	mm	0.00	2.98	135.0	9.66	324.2	1,634
AT	-	°C	-9.50	15.0	31.5	9.34	62.3	1,634
WS	-	m/s	0.40	1.71	5.30	0.74	43.3	1,634
RH	-	%	23.9	68.7	99.0	14.6	21.3	1,634
SR	-	MJ/m^2	0.0	14.1	32.1	7.06	50.1	1,634
E	-	mm	0.29	3.66	9.60	2.02	55.2	1,634
Flow	WJ	m^3/s	0.09	0.68	27.7	1.89	276.9	1,634
	HN		0.22	1.21	36.7	2.65	219.6	1,634
	JS		0.00	0.16	8.91	0.53	336.9	1,634
	PYJ		0.24	1.69	70.0	3.75	221.6	1,634
SS	WJ	mg/L	1.73	25.1	244.0	33.6	133.6	121
	HN		3.21	28.8	236.4	39.0	135.5	109
	JS		3.35	100.2	1,110.0	209.1	208.8	109
	PYJ		1.70	25.1	384.6	43.7	174.1	229
TN	WJ	mg/L	0.08	2.29	6.52	0.83	36.1	121
	HN		0.98	2.39	7.86	0.87	36.3	109
	JS		1.17	3.01	6.72	0.84	27.8	109
	PYJ		0.70	2.19	5.74	0.69	31.4	229
TP	WJ	mg/L	0.01	0.17	1.70	0.16	94.0	121
	HN		0.04	0.18	1.13	0.13	72.7	109
	JS		0.02	0.20	0.82	0.12	61.2	109
	PYJ		0.04	0.14	0.72	0.10	69.1	229

* WS: Study Watershed, ** Std. Dev.: Standard Deviation, *** CoV: Coefficient of Variation.

Table S5. Information use efficiency achieved by ML models trained with the different combinations of training data sets (unit: none or fraction). The highest efficiency statistics are in bold.

ML Models	Training Data Sets	Marginal entropy				Transfer entropy			
		Flow	**SS**	**TN**	**TP**	**Flow**	**SS**	**TN**	**TP**
RF	WD+UC	0.009	0.003	0.011	**0.023**	**5.583**	1.645	**4.674**	2.473
	WD+C	**0.017**	0.002	**0.025**	0.021	1.240	1.046	2.994	**4.161**
	All	0.014	**0.015**	0.012	0.017	1.571	**2.137**	3.368	1.562
SVM	WD+UC	0.031	0.062	0.012	0.019	**9.222**	**3.913**	1.807	2.936
	WD+C	**0.048**	**0.140**	**0.031**	**0.036**	4.033	3.527	**2.825**	**7.264**
	All	0.027	0.061	0.016	0.030	2.046	3.654	2.174	3.435
ANN	WD+UC	0.010	0.021	0.041	0.021	0.777	2.004	2.215	0.564
	WD+C	**0.018**	**0.074**	**0.070**	**0.053**	**1.470**	**2.033**	**4.453**	**3.007**
	All	0.011	0.036	0.033	0.031	0.968	1.513	4.063	2.417

Table S6. Summary statistics of transfer entropy of the training data sets by the watersheds with different machine learning algorithms.

Watershed	Training Data Sets	Flow			SS			TN			TP		
		RF	**SVM**	**ANN**	**RF**	**SVM**	**ANN**	**RF**	**SVM**	**ANN**	**RF**	**SVM**	**ANN**
WJ	WDO	0.299	0.315	0.265	0.385	0.210	0.174	0.215	0.240	0.276	0.174	0.281	0.246
	WD+UC	0.304	0.348	0.451	0.190	0.297	0.214	0.223	0.214	0.388	0.207	0.314	0.315
	WD+C	0.394	0.486	0.485	0.294	0.415	0.381	0.263	0.327	0.312	0.210	0.335	0.340
	All	0.424	0.529	0.469	0.535	0.539	0.514	0.253	0.315	0.324	0.404	0.367	0.349
HN	WDO	0.290	0.328	0.378	0.282	0.173	0.125	0.251	0.173	0.167	0.349	0.375	0.101
	WD+UC	0.395	0.345	0.467	0.291	0.449	0.218	0.325	0.284	0.323	0.382	0.533	0.535
	WD+C	0.439	0.509	0.457	0.461	0.433	0.432	0.312	0.420	0.274	0.387	0.488	0.456
	All	0.472	0.637	0.535	0.527	0.536	0.487	0.387	0.528	0.353	0.620	0.598	0.606
JS	WDO	0.354	0.355	0.333	0.333	0.225	0.213	0.368	0.379	0.173	0.365	0.258	0.137
	WD+UC	0.337	0.415	0.451	0.358	0.325	0.423	0.403	0.499	0.370	0.435	0.364	0.370
	WD+C	0.481	0.470	0.482	0.447	0.511	0.394	0.485	0.531	0.439	0.409	0.343	0.285
	All	0.502	0.589	0.567	0.375	0.424	0.527	0.425	0.558	0.411	0.443	0.466	0.424
PYJ	WDO	0.314	0.386	0.376	0.345	0.358	0.191	0.281	0.351	0.400	0.285	0.337	0.218
	WD+UC	0.432	0.459	0.496	0.455	0.419	0.311	0.446	0.454	0.534	0.526	0.430	0.475
	WD+C	0.417	0.429	0.449	0.402	0.450	0.361	0.316	0.400	0.461	0.413	0.358	0.355
	All	0.479	0.581	0.596	0.588	0.563	0.490	0.403	0.457	0.531	0.524	0.461	0.439